IPST Technical Paper Series Number 583

A Critical Review of Computer Modeling of Kraft Recovery Boilers

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June 1995

Submitted to
TAPPI Engineering Conference
September 11–14, 1995
Dallas, Texas

A CRITICAL REVIEW OF COMPUTER MODELING OF KRAFT RECOVERY BOILERS

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ABSTRACT

This paper assesses the state of technical development of computational fluid dynamics (CFD) based recovery boiler models in the context of what such models are asked to do. Useful models must provide information relevant to fouling and plugging, air emissions, boiler integrity issues, and combustion stability. The critical model outputs needed are

- amount of physical carryover;
- furnace exit gas temperature distribution;
- furnace exit gas velocity distribution;
- wall heat flux distribution;
- amount, size and composition of aerosols from the furnace;
- concentrations of air emission gases;
- bed size, shape, surface temperature distribution, and burning rate distribution;
- some measure of bed stability and "goodness"; and
- overall reduction efficiency.

Many of these outputs already can be predicted. There remain some critical technical enhancements that need to be made to current models. These include drop burning models that are appropriate for recovery furnace conditions, models of aerosol formation in the furnace, good bed models with shape-predicting capability, and effective wall process models. Bridges must be developed that would relate the output of furnace models to the effects on convective section fouling and plugging. Recovery boiler models have reached a point where they can be a useful tool in improving recovery boiler designs and operation. There is a need for benchmarking existing recovery boiler models against each other by devising some agreed-upon cases for each to solve and compare results. The most effective way of using models is to get them in the hands of the stakeholders, boiler manufacturers and companies with kraft pulp mills.

INTRODUCTION

In the last few years, considerable effort has gone into the development of computational fluid dynamics (CFD) based recovery boiler models and the application of these models to improve recovery boiler operation and design. These models are now becoming recognized as engineering tools for evaluating design alternatives rather than just an R&D novelty. It is appropriate to assess the current state of the art of recovery boiler models and to determine what are the critical tasks that still need to be accomplished to make recovery boiler models a cost-effective tool for improving recovery boiler performance.

CFD-based recovery boiler models were first developed in the latter part of the 1980s. [1,2] They drew on a large amount of new fundamental information on black liquor combustion that was generated in the 1980s as well as the availability of CFD programs that could solve complex flow problems. The initial focus of these models was on the prediction of the amount of physical carryover of burning black liquor and smelt out of the furnace cavity, since this was felt to be the most important factor governing fouling rates. The impetus to use models as a tool was enhanced by the large number of recovery boiler retrofits to gain liquor burning capacity that were carried out in the 1980s. In 1990, a large Department of Energy (DOE) supported program to develop recovery furnace models, involving the Institute of Paper Science and Technology (IPST), the University of British Columbia (UBC), and Oregon State University (OSU), was begun and is continuing. [3] During this same period, essentially all of the recovery boiler manufacturers have developed recovery boiler models as a design and troubleshooting tool.

The objective of this paper is to assess the state of the art of recovery boilers in the context of what such models need to do. A review will be made of the type of information needed to improve recovery boiler operation and the capability of existing recovery boiler models, especially furnace models, to supply this information. Gaps, where additional fundamental information is needed or where models are lacking, will be identified. The impediments to more extensive use of models will be noted and means for overcoming these impediments suggested. Critical areas requiring further work will be delineated.

USE OF RECOVERY BOILER MODELS

Recovery boiler models are not an end in themselves. The need is for an effective problem solving tool, not for "virtual reality" recovery boilers. Use of recovery boiler models must lead to improvements in recovery boiler operation and design and serve as a means for increasing the general understanding of recovery boiler operation.

Potential users of recovery boiler models can be divided into four broad classes: boiler manufacturers, kraft pulp producers operating recovery boilers, service firms providing engineering and consulting, and academic institutions. Each of these potential users has different needs and expectations.

Boiler manufacturers are the most likely source of recovery boiler process improvements. Boiler manufacturers use models for process insight to guide design changes and for guidance in troubleshooting operating problems. Models are being used as a sales tool to increase credibility with customers. Good recovery boiler models could provide a means for gaining a competitive advantage over other boiler manufacturers. Models have already been used for determining optimum air port arrangements and for evaluating changes in liquor firing practices.

Kraft pulp mills could use models to guide evolutionary changes to improve recovery boiler productivity and for troubleshooting operating problems. A typical application would be to determine how changes in operating procedures and/or hardware modifications would provide gains in liquor burning capacity in existing units. Models could also be used in developing recovery boiler specifications or for assessing the capabilities of proposed equipment. In general, kraft pulp manufacturers benefit from good models in the hands of the boiler manufacturers. At the present level of technical complexity, CFD-based models are probably beyond the scope of individual kraft mills and would require corporate level support for application. This could change in the future.

Engineering firms and consultants could use models for troubleshooting operating problems and in evaluating proposed equipment. At present, there has not been great interest shown by such service firms in obtaining access to CFD-based recovery furnace models.

Academic institutions have been involved in the development of recovery boiler models, but their role in model use is less obvious. One possible role would be to use models to develop a general understanding of how recovery boilers operate.

Information Needed on Recovery Boilers

In order to improve recovery boiler performance, it is necessary to understand the effects of furnace design, furnace operating variables, and liquor quality on the following:

1. fouling and plugging rates,
2. air emissions,
3. combustion stability and bed control,
4. corrosion and other boiler integrity issues,
5. steam and electric power production, and
6. reduction efficiency.

The overall challenge is to define optimum operating strategies (liquor spray and air entry conditions) which will maximize liquor firing rates while

- achieving acceptable plugging rates,
- meeting air emission restrictions, and
- maintaining a safe, stable operation.

Information Models Can Provide

Having defined the information needed about recovery boilers, we next need to look at what models can provide and what they cannot. Each of the six categories of information needs listed above are discussed in the following.

Fouling and plugging.

Fouling of heat transfer surfaces and plugging of gas passages is the factor that ultimately limits firing rates on most recovery boilers. The material that causes fouling and plugging is usually divided into two classes; carryover and fume or dust.

Carryover is the name given to the macrosized remnants of burning liquor drops that are physically entrained in the gas stream leaving the furnace and carried into the convective sections of the boiler. These macrosized particles easily impact on the windward side of heat transfer surfaces and can freeze on tubes and form hard deposits. They have generally been considered a prime cause of plugging and the conventional wisdom is that carryover should be minimized.

Current CFD-based models can predict the amount, chemical composition, and physical state of the carryover material. Carryover prediction was a prime motivation for the original development of such models and is one of the most useful model outputs. In addition to the amount, chemical composition, and physical state of the carryover material, other factors may influence boiler plugging by carryover deposits. These include gas velocities, gas temperature, gas composition, furnace geometry, and sootblowing practices.

Fume or dust is the name given to the very small (micron-sized) particles produced by vaporization and condensation processes in the furnace. Recent experience indicates that many, if not most, recovery boiler plugging problems involve dust deposits. Thus, for recovery boiler models to deal effectively with plugging problems, they must be able to deal with dust deposits. Unfortunately, the factors influencing dust deposition rates, deposit hardening, and deposit removal are not well-understood. The amount of dust leaving the furnace cavity, dust size, dust composition, gas velocities, gas temperatures, gas composition, convective section geometries, and metal temperatures may all be important factors. Current furnace models do not have the capability of predicting the amount, size, and composition of the aerosols leaving the furnace. Furnace models do have the capability of predicting the distribution of gas velocities and temperatures out of the furnace. Current models do not have the capability of predicting all of the gas concentrations that might be relevant to deposit formation and hardening, but this capability is becoming available.

There is a clear need to develop bridges that would relate the output of furnace models to the effects on convective section fouling and plugging. It is recognized that peak furnace exit gas temperature is an important parameter, but there are undoubtably others. It is also likely that furnace models may have to be enhanced to provide the capability of predicting the key information needed.

Air emissions.
Air emission constraints can limit recovery boiler operation. Thus useful recovery boiler models should have a capability of predicting the effects of operating changes on air emissions. Even if models prove incapable of accurately predicting absolute levels of each emission-limited substance, they should be capable of dealing with the effects of changes and with trade-offs between different substances that might have emission limits.

Of the gaseous emissions potentially subjected to limits, TRS, CO, and VOCs are all substances that are destroyed by oxidation. The destruction of these materials is essentially a stoichiometry and mixing issue. There may also be some kinetic limitations at lower temperatures. Current models are capable of predicting CO emissions. As a first approximation, other oxidizable substances could be proportioned to CO. More elaborate models with separate kinetic limitations could be used if necessary.

The fundamental chemistry by which SO_2 is converted to sulfates within the furnace is becoming understood as are the factors that govern sulfur release from the burning liquor drops. [4,5] Algorithms for modeling SO_2 concentrations from the furnace should be available within the next year.

Considerable information on NO_x formation and destruction has been published within the last year, and algorithms for predicting NO_x in recovery boilers should be available within the next year. [6,7]

The basic information for predicting HCl concentrations is now available. [8] Since HCl formation depends on SO_2 concentrations, predictions of HCl concentrations require simultaneous prediction of SO_2.

The prediction of particulate emissions and/or opacity is more complicated. Particulate emissions depend on both the dust load and the precipitator collection efficiency and are, in fact, dominated by the precipitator performance. Furnace models have the potential for predicting dust loads (although this has not yet been implemented). There are no plans to model precipitators in current modeling programs.

Combustion stability and bed control.
Unstable combustion is potentially hazardous. Operating conditions that are conducive to blackout, either local blacking out of primary air ports or a more general loss of fire, should be avoided. There is usually a close link between combustion problems and char bed behavior. Unstable char beds are often the main manifestation of combustion instability.

Although bed control is an important issue, it is one that is hard to quantify. There is a need to define what constitutes a "good" bed. This is a somewhat subjective matter involving bed size, shape, surface temperature, burning rates, and stability. There are two factors that currently limit the ability of models to deal with these issues. One is a lack of an adequate bed model. The other is the lack of consensus on what constitutes a "good" bed, especially in a quantitative sense.

Auxiliary fuel usage can be effective in dealing with unstable char beds. This is currently not being modeled. The assumption is made that an optimum recovery boiler should be operating autogenously on black liquor.

Corrosion and boiler integrity.
Although corrosion, tube cracking, and other boiler integrity issues are critical to safe operation, they have not been a major focus of modeling. This is mainly because of a lack of sufficient understanding of the key underlying processes, but also because at least some of these issues are not amenable to attack with steady-state furnace models.

Corrosion generally depends on three factors: local chemical environment, metal temperature, and metallurgy. Models have some capability of addressing the first two issues, but only in a limited fashion.

Furnace models have the potential for predicting the heat flux distribution to the waterwalls. The heat flux has an effect on metal temperatures (along with boiler pressure, circulation, and waterside deposits). In general, areas of higher heat flux would be more likely to have higher corrosion rates. Avoidance of local areas of high heat flux could be a criterion in seeking to optimize furnace performance.

Furnace models can predict the composition of some of the furnace gases that might be involved in corrosion. There is a problem in accurately predicting gas concentrations very close to a boundary without introducing an excessive number of computational elements. A more serious problem is that the relevant chemical environment is the one that exists at the metal surface, and this surface is covered by frozen smelt and/or char. The relationship between furnace gases and the local environment at the metal surface is not currently understood.

Steam and power production.
CFD-based models are overkill as far as steam production is concerned. Steam efficiencies are determined by heat balance considerations and are dominated by externalities. Air emission constraints tend to require complete combustion, so unburned fuel in gases is not a significant issue. The main variables affecting steam efficiency that could have some relevance to models are the amount of excess air and the amount of residual carbon in the smelt. The latter quantity might be an output of a good bed model.

Power production is affected by steam temperature and so is affected by the performance of the superheater. The extent of superheater fouling is probably the most important factor influencing steam temperature. Carryover would be expected to be significant here, and carryover predictions are amenable to modeling. In addition, the furnace exit gas temperature and velocity distribution should be important and this is also amenable to model prediction. However, cleaning processes are also important and this is not addressed by models.

Reduction efficiency.
Reduction efficiency is another parameter important to recovery boiler operation, although reduction efficiency has little economic significance once values in the +90% range are achieved. The overall reduction efficiency is dependent on the amount of reduction that takes place during black liquor pyrolysis and char burning and also on the amount of smelt reoxidation that occurs before the smelt flows out of the furnace. The sulfur chemistry during black liquor pyrolysis is becoming understood. New rate equations for sulfate reduction by carbon are available and have been incorporated in some black liquor burning models and char bed models. [9] Thus, the capability to predict overall reduction efficiencies with furnace models is nearly in hand. Good bed models and good models of wall processes are necessary to do a good job of predicting reduction efficiencies.

Summary of critical information.
Based on the analysis above, the furnace model outputs that are most critical as a tool for improving furnace performance are

- amount of physical carryover;
- furnace exit gas temperature distribution;
- furnace exit gas velocity distributions;
- wall heat flux distributions;
- amount, size, and composition of aerosols from the furnace;
- concentrations of air emission gases;
- bed size, shape, surface temperature distribution, and burning rate distribution;
- some measure of bed stability and "goodness"; and
- overall reduction efficiency.

TECHNICAL CRITIQUE OF FURNACE MODELS

The previous section defined the information that CFD-based recovery boiler models are being asked to provide. The next step is to look at existing models from a technical standpoint to assess the degree that they are capable of providing the necessary information with reasonable accuracy and to define those areas where more development is needed.

Recovery boiler models generally consist of two parts: a CFD part and a black liquor combustion model. These two parts are coupled to provide the complete model. The CFD part solves the gas mass, momentum, and energy equations to provide gas velocity, temperature, and concentration fields. The black liquor combustion models interact with the gas fields and provide source/sink terms to the CFD equations. Black liquor burning rates depend on the gas fields and, in turn, influence them through the source/sink terms.

Some recovery boiler models are limited to the furnace cavity itself and are terminated at the nose arch. Others carry flow and temperature calculations through the superheater. Still others carry the model through the furnace and the entire convective section. This discussion basically will be limited to the furnace.

CFD Adequacy

Various CFD code platforms are in use for recovery boiler models. Some are based on the commercially available CFD codes, such as FLUENT and PHOENICS. Others, such as the model being developed at UBC and a model at Babcock & Wilcox, are based on internally-generated CFD codes. One of the technical issues is the adequacy of these various CFD platforms for recovery boiler models. Do these codes give reasonable predictions of recovery boiler flows and the temperature and concentration fields? Do different CFD codes give similar results when applied to the same problem?

At the present time it appears that the CFD codes are adequate for predicting the gas flows in the furnace. There have been limited attempts to compare predicted flows with measured flows, and the agreement has generally been reasonable. Most of these comparisons have been done in isolation to verify the applicability of a particular code. There would be considerable value in comparing the ability of different CFD codes to predict the flow for the same cases in a benchmarking exercise. This would add to the credibility of CFD predictions of recovery boiler flows and help pinpoint areas of weakness in flow prediction.

Empirical turbulence models are needed in the CFD models, and the specific turbulence models used do have an effect on flow predictions. This is another area where benchmarking could prove useful. There is a need for a consensus on what is adequate for a turbulence model for recovery boiler flows.

Gas flows in recovery boilers are not necessarily stable, as has been shown both with CFD model calculations and by experimental measurements. This has an effect when steady-state solutions to the CFD equations are sought. When flows are unstable, the CFD calculations stall out at high residuals. If a transient case is then run, movement of the core flow can be seen. There are some indications that flows with circulation tend to be more stable.

It is not clear that unstable flows are inherently bad and should be avoided. If unstable flows do not have to be avoided, it is necessary to develop means for dealing with unstable flow fields. Time-dependent solutions constitute an enormous calculation burden and are clearly not the answer. The time-average of an oscillating flow may not have the same properties as the actual unstable flow and may also not be the solution produced by the CFD code. This remains an open issue.

Considering all the available information, current recovery boiler models appear to adequately handle flow predictions. Flow prediction does not appear to be the area with the greatest uncertainty, at least with respect to the information needed to improve recovery boiler performance.

Limited comparisons between computed hot flow patterns and isothermal flows (at an appropriate average gas temperature) have been made, and these have tended to show reasonable similarity. [10] Differences between hot flows and isothermal flows come from volume flow sources and sinks. There are three sources/sinks for volume flow that result from black liquor combustion. These are

- evaporation of water from the black liquor;
- gas mole changes resulting from black liquor combustion; and
- density changes associated with temperature gradients.

In many cases, these volume flow source/sinks perturb, but do not dominate, the flow patterns. One area where this may not be the case is the flow in the superheater, where the gas density changes associated with temperature changes from heat absorption can induce recirculating flows.

The ability to accurately predict gas temperatures depends on the ability to predict heat transfer rates to the waterwalls and properly handling all chemical reactions. There are some indications in published hot flow model results that gas temperature predictions in the lower furnace may be too high. Several papers have indicated gas temperatures in some regions in excess of 1600°C. [11,12] It is not evident that such high temperatures have ever been measured in a recovery boiler. This may be an indication that significant endothermic reactions are being neglected or that calculated gas reaction rates are too fast.

The ability to properly predict gas concentrations is merely a matter of putting in the proper stoichiometric relations and rate equations for the particular species in question. The CFD codes may put limits on the number of gas species that can be handled. If this is the case, then certain species cannot be predicted. One way around this problem is to consider only the main gas species that affect the mass and energy balances when doing the iterative CFD calculations of the gas fields. The minor constituents can then be calculated from a second, simpler model which uses fixed gas flow, temperature, and concentration fields.

Black Liquor Modeling

The black liquor combustion model is the second major component of a recovery boiler model. Black liquor burns in a number of different ways in the recovery furnace: as drops in flight, on the char bed, and on the wall. All of these must be accounted for in a recovery boiler model. At the present time, there is more uncertainty with respect to how the black liquor behavior should be modeled than there is with the CFD component of recovery boiler models.

Drop trajectory models.

Black liquor is sprayed into the furnace as rather coarse drops which pass through the furnace gases and dry and burn as they move. The liquor drops eventually land on the hearth, reach a furnace wall, or are carried out of the furnace with the gases. The trajectories that individual drops follow are determined by initial vector velocities, gravity, and fluid drag. Trajectory models must account for the changes in mass and physical size of the drops as they burn. Current methods for calculating drop trajectories by force balance are adequate. The biggest uncertainties are associated with the proper assignment of initial velocities and drop sizes, and with the empirical treatment of the swelling and deswelling that accompanies liquor burning.

Another factor affecting trajectory calculations is whether a deterministic or stochastic trajectory model is used. The scale of turbulence is such that it can affect trajectories. Some models use the average gas velocity in a given computational cell for determining the drag on the liquor drop while it is in that cell. Every drop passing through a particular cell is exposed to the same velocity. Other models use a probablistic turbulent velocity component added to the average gas velocity in determining the drag. In this case, all drops that start out with the same conditions do not end up in the same place. Trajectory calculations directly determine the amount of carryover. Unpublished simulations have shown, at least for a gas flow pattern with a strong central updraft, that the amount of carryover calculated can differ significantly between these two calculation methods.

Drop burning models.

There has been considerable improvement in black liquor burning models over the years. The initial models treated the liquor as containing four substances: water, volatiles, char carbon, and ash. These early models are sometimes referred to as "earth, air, fire, and water" models. They were adequate for describing the weight changes and volumetric changes occurring during burning needed for trajectory calculations and carryover prediction. They are inadequate for proper calculation of the source/sink terms needed to predict hot flow fields. Black liquor drop burning models are now available which give rate equations for the transfer of individual elements in the liquor to the gas phase. These models also include a proper treatment of char gasification as well as oxidation. These elemental transfer models have been or are now in the process of being incorporated into the drop burning models. They provide a much better basis for proper modeling of source/sink terms.

One of the most critical remaining problems is to develop and verify drop burning models specifically for recovery furnace conditions. [13] Existing drop burning models are based on laboratory experiments. Most of these have been carried out with black liquor drops suspended in muffle furnaces. Others have been carried out in laminar entrained flow reactors. One issue is a proper description of the rate processes that depend on the particular environment in which the drop is present. Another is defining the stoichiometric partition factors and swelling factors that now are empirically linked to variables in the laboratory setups that do not have an obvious counterpart in the furnace. There remains a need to have an experimentally validated drop burning model that involves only those variables that are meaningful in a CFD furnace model.

Another issue is how to deal with liquor-dependent parameters. The swelling tendency of a liquor depends on composition. Measurements of swelling made in the laboratory under arbitrary conditions can be used as a basis for describing swelling in the furnace, but there is a degree of uncertainty involved. It is known that individual sulfur compounds in the black liquor behave differently during pyrolysis, and this can affect the extent of reduction during pyrolysis and sulfur release to the gas phase. [5] Unpublished laboratory data have been obtained that show significant liquor to liquor variations in sodium release. It is not yet certain how important this is under furnace conditions and how to deal with it in the models.

Char bed models.

The best current char bed models are capable of describing burning rates and interactions with the gas fields above the bed. However, there is no doubt that better char bed models are needed. Improvements are needed in treatments of surface and subsurface burning rates. There is also a need to have a means for predicting bed shape and stability. Several boiler manufacturers have indicated that they consider the ability to predict bed shape to be critical.

There is an inherent dichotomy in using a steady-state furnace model to predict bed shape, since there is no guarantee that bed burning rates match the rate at which material is delivered to the bed. Some modelers have addressed this issue by arbitrarily assuming a bed shape and then assuming that everything that reaches the bed burns (as it must at steady state). While this approach may allow closure of energy balances and not greatly affect predictions of gas conditions leaving the furnace, it certainly begs the question of combustion stability and whether the operating conditions being modeled are actually feasible.

A proper bed model must allow a predicted bed geometry to be an outgrowth of the bed model integrated to the above bed burning. It must not only provide bed burning rates, it should also allow for accumulation and depletion of material and physical transport of char along and off the bed surface in arriving at the ultimate size and shape.

The chemical basis for modeling bed burning rates is available. It is essentially the same as that used in the char burning step in the drop model. Char gasification by CO_2 and H_2O is included along with oxidation of product gases in the boundary layer in a combined mass transfer - chemical kinetics limited burning. Carbon consumption by reaction with sodium sulfate and carbonate can also be included. These latter reactions can occur subsurface.

Effective means for providing for redistribution of char by physical transport along the bed surface have not yet been implemented in bed models.

Wall processes.
The liquor drops that strike the walls of the furnace wall must be treated in a realistic manner. A variety of ways of handling liquor which reached the walls were used in early recovery boiler models. For example, when models were used only for carryover predictions, liquor which struck the walls was usually ignored. Another technique (not very realistic) was to assume that a liquor drop that reached the wall bounced off. A more sophisticated way of handling wall processes, and one that did allow a steady state solution, was to assume that a particle that reached the wall continued burning at the same rate that it was burning at just before it reached the wall until all of the fuel was gone.

A realistic wall burning model must allow for the fact that, in the furnace, liquor accumulates on the wall and then periodically sluffs off and falls to the bed. This can, in fact, be a very significant way that fuel and inorganic reach the bed. Recently, one boiler manufacturer has developed a wall model that treats the liquor burning rate on the wall in a similar manner to the burning rate on the char bed. If there is an inbalance between the rate at which liquor substances reach the wall and the burning rate, the excess is assumed to sluff off and fall to the bed. [13] This appears to be a reasonable way of treating wall burning.

Liquor spray models.
Liquor sprays are modeled by setting up the initial conditions at which liquor drops enter the boiler. The key issues with liquor models are whether or not the finite length required to form drops should be dealt with and how to relate the drop specifications to the nozzle geometry and the actual variables (flow, liquor temperature, etc.) available to the operator. It is unclear whether or not spray distribution data obtained under laboratory conditions are relevant to sprays formed in the high-temperature environment of the furnace.

Heat transfer models.
There appears to be considerable uncertainty and disagreement with regard to how to handle radiant heat transfer in the furnace. Much of this has to do with the effect of fume and other furnace aerosols on radiation heat transfer. Some people believe fume may act like soot. Others consider it a minor matter.

It appears that there are good radiation models available. What is lacking is reliable data for radiation properties in a recovery boiler environment. This need is being specifically addressed in the extended DOE recovery boiler modeling project. Babcock & Wilcox is a subcontractor on this project to obtain data on critical properties that affect radiative heat transfer in black liquor combustion and to develop strategies for accurate treatment of heat transfer in recovery boilers.

Fouling and plugging models.
This is a gap area. Additional information needs to be obtained and integrated into a cohesive view of plugging processes in the furnace. It is probably not necessary to develop a mathematical model of the fouling process. What is actually needed is a bridge between what a furnace model is able to predict and the consequences in terms of fouling and plugging the convective sections. The effects of the amount, size, and composition of aerosols on plugging must be understood. It is also necessary to be able to interpret quantitatively how gas temperature, gas velocity, gas composition, and chemical reactions affect deposition rates and hardening. The essential question to be answered is "how does furnace operation (i.e. how black liquor and air are put into the unit) affect fouling and plugging?"

One critical need is to define the nature of the aerosol forming processes in the recovery boiler. A wealth of new information was presented at the 1995 International Chemical Recovery Conference. [14,15,16] This has to be interpreted. Sintering and hardening of deposits is also an essential element of the plugging and fouling process. There is considerable laboratory data on sintering and hardening rates as a function of composition. There is a need to tie this behavior more closely to field conditions.

Removal of deposits from heat transfer surfaces is an absolutely essential element of the plugging and fouling process. Recovery boilers would probably plug within 24 hours after liquor firing was initiated if sootblowers were not used. Thus, considerations of deposit removal must be incorporated into the information bridge between furnace models and fouling and plugging of the upper furnace.

Excellent work on aerosol formation, deposition, hardening, and removal is being carried out at the University of Toronto, Åbo Akademi, VTT in Finland, Oregon State University, and at boiler manufacturers. This can be used to address fouling and plugging issues.

Corrosion models.
Modeling of corrosion processes in recovery boilers, as part of more general recovery boiler models, is probably not feasible at this time.There are no plans for modeling corrosion in the DOE project.

Application Issues

There are many impediments to the effective use of recovery furnace models. These include:

- the high computational intensity of calculations,
- the high degree of skill needed to set up problems and guide convergence,
- limited correspondence between the type of information needed to solve recovery boiler problems and the type of information a furnace model can produce,
- the immense amount of information developed by the models must be distilled and condensed and presented in a manner that the user can understand it,
- the inefficiency in re-solving the entire recovery boiler furnace field to see the effects of changing a single parameter, and
- the lack of confidence in the reliability of model predictions.

Overcoming these impediments presents many challenges.

Using faster, bigger computers may not be the only or even the best answer to the issue of high computational intensity. There is a clear need for simpler models to provide most of the answers sought, with full-blown models used only for confirmation purposes.

Compromises must sometimes be made in setting up a problem in order to describe the boiler geometry in a reasonable number of computational cells or elements. This may result in air ports being moved in the model to fit grid lines lined up with other ports. Air port openings in the model may be larger than the real ports in order to fit a grid. This can be dealt with by introducing a port porosity, but this will affect predicted flows. Primary ports are usually modeled as slots in order to keep the computational nodes reasonable. This usually has a minor effect on the flows, but it could influence bed burning rate predictions, especially close to the walls.

CRITICAL ISSUES

In September 1994, a symposium on recovery boiler modeling was held involving model developers, boiler manufacturers, and kraft pulp manufacturers. A summary of what model users felt were the most critical things needed is given below:

- model validation,
- good bed models,
- wall interactions models,
- fume, NO_x,and S chemistry models,
- definition/criteria for stable combustion,
- radiation in dense, reacting, particle-laden flows, and
- how to define an optimum furnace.

It was generally agreed that it would be of great value to set up a program to benchmark various recovery boiler model codes against one another. If this benchmarking effort resulted in general agreement, it would add greatly to model credibility. Where there were differences in model predictions, it would help point out critical issues that needed to be addressed. There was a general consensus that radiation and turbulence were not handled that well with current recovery boiler models.

Technology Transfer

It is clear that the benefits of recovery boiler models will only be fully realized if the models, submodels, approaches, etc., get into the hands of those who have a stake in improving recovery boilers and know enough about them to use the models effectively. In general, these are the boiler manufacturers and companies operating kraft mills.

There is also a need to use models to develop a better understanding of how boilers operate and provide general guidelines on firing practices and air supply. One of the long-range goals of the recovery boiler modeling effort is to provide guidelines for optimum liquor spray arrangements and air entry conditions. This might most appropriately be done through a series of simulations on a generic recovery boiler chosen for computational efficiency and ease of systematic altering of key parameters. Academic institutions might play a role here. It will be difficult to come up with general conclusions from isolated cases on individual boilers done on a piecemeal basis.

Credibility

Finally, there is the challenge of model validation. This is essentially an issue of users having confidence in the predictions of the model. Validation has been an ongoing part of the model development effort. Isothermal model calculated flows have been tested against data from water flow models of two different recovery boilers with reasonable success. Model predictions have also been compared against limited cold flow data in recovery boilers. The results of these efforts indicate that overall flow predictions are reasonable. The black liquor combustion models that are being developed have been validated against single-drop black liquor burning data from laboratory systems.

It is clear that the global furnace model must also be validated against field data obtained on actual recovery boilers. Validation will be based on a comparison between model-predicted and measured results of cause-and-effect relations between selected operating variables and critical output variables. Thus, validation will be intimately tied to what the models will be used for. Model validation at this level is not seen as something that requires breakthrough developments in sensors and measurement technology on recovery boilers. The necessary measurements can be made with existing methods, especially if the measurements need only be made for a limited time.

One boiler manufacturer plans to validate its model first against lab data and then with a pilot recovery boiler. Another has done full-scale cold flow measurements on a recovery boiler at a mill. They saw the same features in the flow that had been seen in earlier CFD calculations on that boiler.

Every successful application of a recovery boiler model adds to credibility. Careless use of models for situations for which they are not appropriate can only destroy credibility.

CONCLUSIONS

Recovery boiler models have reached the point where they can be an effective tool in improving recovery boiler performance if they are used properly. The biggest current uncertainties are on the black liquor modeling side. The information for dealing with these uncertainties is in hand or being developed and these problems should be overcome in the very near future.

The most effective way of using models is to get them in the hands of the stakeholders, boiler manufacturers and companies with kraft pulp mills.

There is a need for benchmarking existing recovery boiler models against each other by devising some agreed upon cases for each to solve and compare results.

There are some critical technical enhancements that need to be done to existing models:

- drop burning models that are appropriate for recovery furnace conditions,
- models of aerosol formation in the furnace,
- good bed models with shape predicting capability, and
- effective wall process models.

Since most applications eventually deal with boiler plugging, the understanding needed to relate model predictions to plugging parameters must be obtained. A bridge between the predictions of a recovery furnace model and the effect on boiler plugging must be developed. There is an immense international effort on this subject right now that should bear fruit.

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ACKNOWLEDGEMENT

This paper is based on work supported by the U.S. Department of Energy, Office of Industrial Technologies under DOE contract no. DE-FG02-90CE40936.